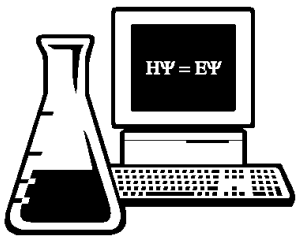
AMPAC 6.0

User's Manual Addendum

A Product of:



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What's New in AMPAC 6.0?

AMPAC Computational Module:

- New larger and more efficient CI
- More accurate and faster geometry optimization
- More accurate and faster SCF convergence
- Better memory usage
- COSMO solvation model
- MNDO/d semiempirical model

AMPAC Graphical User Interface:

- Expanded Builder options
- Full support for Gaussian94®
- Surface displays (MOs, ESP)
- UnDo / ReDo
- Submit and manage jobs from the interface
- Redesigned Z-Matrix editor
- Clean function for initial geometry optimization
- Redesigned AMPAC and Gaussian dialog boxes

Introduction

This manual is intended to serve as a supplement to the *AMPAC 5.0 User's Manual*. You will need the 5.0 manual to successfully use this addendum. If you have misplaced the copy that came with your program or need additional copies, these can be obtained from Semichem at a minimal cost. The structure of this addendum is as follows:

Chapter 1 Errata: Corrections to the *AMPAC 5.0 User's Manual*

Chapter 2 Corrected Keywords Arranged by Computational Task

Chapter 3 New Functions and Keywords Arranged by Computational Task

Chapter 4 New AMPAC Utilities

Chapter 5 New References

Chapter 1: Errata: Corrections to the *AMPAC 5.0 User's Manual*

Please refer to your *AMPAC 5.0 User's Manual* for page and section references in this chapter.

- **Page 16**: Elements for AM1

  add: As, Se, Sb, Te

  delete: Ga

- **Page 16**: Elements for PM3

  delete: B

- **Page 82**: The TV must come from an LTRD calculation, not FORCE

Chapter 2: Corrected Keywords Arranged by Computational Task

Listed in this chapter are existing keywords that have changed meaning and/or function from AMPAC 5.0. Please refer to the *AMPAC 5.0 User's Manual* for page numbers and section references.

SCF Control

FILL In an RHF calculation, the initially computed molecular orbitals are used as prototype molecular orbitals for the remainder of the calculation.

FILL=n In an RHF calculation, force MO #n to be the last MO filled with electrons.

FILL=(n,...) In an RHF calculation, force MOs #n, ... to be the last MOs filled with electrons.

OCTET Specifies a spin state with seven unpaired electrons.

NONET Specifies a spin state with eight unpaired electrons.

DECET Specifies a spin state with nine unpaired electrons.

XX-ET Specifies a spin state with (XX-1) unpaired electrons.

Frequency Computation

FORCE Now only a frequency calculator and works in both Cartesian and internal coordinates.

LTRD Performs a geometry optimization (with full diagonalization of the Hessian at each step) and then invokes FORCE for frequency analysis.

Potential Surface Examination and Geometry Optimization

T.V.=n (This option is used with both PATH and IRC). No longer will the user be required to provide an oriented transition vector. The "n" used

here is the numerical identifier for the vector to be followed by PATH and IRC. By specifying a positive number the mode will be followed "forward". A negative number will follow the mode "backward". This is useful for verifying that a particular mode corresponds to a particular TS on a specific reaction pathway.

IRC=x.x
PATH=x.x

PATH and IRC are now multistage jobs, involving the following steps: 1) Minimize gradients of the geometry by LTRD; 2) Obtain the vector to be eliminated from T.V.=n; 3) Follow steepest descent left and right of the located point. The value x.x defines the distance along the TV that must be traveled before frequencies are computed. It is usually not recommended that this variable be altered, as vast output may result.

Chapter 3: New Functions and Keywords Arranged by Computational Task

Listed here are new keywords and brief descriptions of new functionality found in AMPAC 6.0 that were not included in AMPAC 5.0.

Computational Strategies

All convergence criteria have been enhanced for more general accuracy and reliability. It is not usually necessary that you use SCFCRT=0, GNORM=low value, or PRECISE for routine calculations. Use of these keywords is only needed in VERY difficult situations and may lead to excessively long computation times. *This is a departure from our previous recommendations.*

Visualization Strategies

In this version of AMPAC, Semichem has implemented advanced visualization tools that more closely integrate the program with the Graphical User Interface (GUI) distributed with AMPAC itself. The primary difference the user will note is the presence of .vis files in the directory after calculation. These files contain data that will allow the construction of various surfaces and other options. Most of the data for visualization can still be found in the .out and/or .arc files, but more and more of the information needed for specialized visualization options will come from the .vis file. We recommend that users utilize the .vis file for routine work and examine the text in the output for additional information when needed. Note that the .vis file is a special binary format, but is portable among various computer systems by ftp, if the "binary" transfer option is used. The contents of the .vis file may be dumped in ASCII by using the visdump utility (see Chapter 4).

Semiempirical Methods

MNDOD Invokes the MNDOD method contributed to AMPAC by Professor Walter Thiel at the University of Zurich. Currently included elements are H, Li, Be, B, C, N, O, F, Al, Si, P, S, Cl, Zn, Ge, Br, Sn, and I.

COSMO Solvation Method

COSMO If just the keyword COSMO is specified, the dielectric constant for water is used.

EPS=n.m Performs a COSMO solvation calculation using n.n as the solvent's dielectric constant.

RSOLV=x.x Defines the solvent's molecular radius. The default value is 1.0

REFRACT=x.x Defines the solvent's refractive index. Default is 1.3.

COSMOWRT Writes data for further COSMO post-processing (COSMO-RS) in ASCII the .out file as well as a portable binary file.

SCF Control and Options

QCSCF A new "quadratically convergent" SCF algorithm has been added. The QCSCF method can either be used immediately if called by the QCSCF keyword, or will be automatically invoked if the energy does not decrease quickly enough. The converger is based on MO rotations by exponential transformation, rational functional approximation, and a search for λ by a Davidson-like diagonalization. Control of the stepsize is exercised to ensure a decrease in energy at each cycle.

HYPERFINE Hyperfine coupling coefficients are computed and output for a UHF calculation.

Potential Surface Examination and Geometry Optimization

GRID=n Computes a 2D spirally-generated grid of points about the defined geometry. (The spiral-generation improves the opportunity for a smooth extrapolation for the initial guess for each successive point from the results from previous points.) The number of points long a side of the grid may be specified by the "n" value. The GRID algorithm also provides rough location of stationary points and has been connected to the TRUST geometry optimization algorithm. Use of STEP1= and STEP2= are still required to set the interval between steps in the search.

TRUSTE Minimize energy using the TRUST algorithm. (This method is now AMPAC's default approach.)

TRUSTG Minimize gradient using the TRUST algorithm for transition state refinement. Note that TRUSTG is slower than TRUSTE. (Recommended and encouraged!)

Configuration Interaction (CI)

Note that the perturbative sort algorithm used to select microstates to be retained for diagonalization the CI matrix has been changed significantly to preserve eigenstates that were previously lost when larger CI calculations were performed. This MAY STRONGLY effect the results of your CI calculations. CI on smaller sets (C.I.=6-8) should not change from results using previous versions of AMPAC. However, larger CI calculations may give different results. In summary, the new CI applied to large CI sets will:

- retain more microstates, and thus be more time-consuming
- be more accurate overall
- produce better UV-Visible spectra

If you were working on a project with the CI in AMPAC 5.0, it is probably best to complete it with that version of the program. The new CI in AMPAC 6.0 may yield slightly different results and they are thus not strictly comparable to the AMPAC 5.0 results.

CISTATE= This is the number of states computed in the CI procedure and printed out. The default is ROOT+3.

DYNPOL Produces output for the dynamic polarizability method for computed the polarizability of CI excited states.

MICROS=n Generates only microstates in the output that have spin=n.

MSCHARG=n.n Certain microstates are discarded from the list of microstates used in the CI reduction due to charges exceeding n.n. (This option is used to remove ionic microstates from consideration.)

CIGAP=n.nnnn Specifies the gap that CI uses to determine if two MOs are degenerate. The default value is 0.0001eV.

Simulated Annealing

WHOLE End the quenching step with full optimizations rather than estimates.

WHOLE=XYZ End the quenching step with full optimizations rather than estimates, but perform the optimizations in Cartesian coordinates.

FREF=x.xx Use an energetic window for selection of conformers centered at x.xx kcal/mol. Note that the x.xx value MUST be provided here. This keyword is only active with MANN.

SREF=x.xx Defines the half-width of the FREF window. If not specified, the value of 30 kcal/mol is taken as default.

AUTOLIMIT Augments the capabilities of the LIMIT keyword, in that AUTOLIMIT defines a set of automatic boundaries for searches rather than requiring that the user explicitly define these limits as

when using the keyword LIMIT. The limits set are: bond lengths = ± 0.1 Å and bond angles ± 20°. No limit is place on dihedrals. This will have the effect of retaining chemical bonds and searching for nearby conformers.

Job Control

T= Job timings may now be specified by the use of the "h" for hours and "m" for minutes modifiers. For example: T=3600 is the same as T=1h and T=60m.

IADM Produces an interatomic distance matrix. The default in AMPAC now is NO matrix.

NOVIS Suppresses printing of the .vis file used for advanced visualization with AMPAC's GUI.

Chapter 4: AMPAC Utilities

mampac

Will execute one at a time and in alphabetical order all AMPAC (.dat) files in the current directory. This utility produces a MAMPAC.LOG file summarizing the progress of the AMPAC calculations.

ampdiff

This utility compares AMPAC .out files in one directory to another and reports the differences in results. It is used to verify and installation of AMPAC after the test suite has been executed.

Suggested usage:
ampdiff (ref. directory) (test directory) > file.txt

haltampac

This utility will find the AMPAC jobs currently running over which the user has control and provide the option to halt one or all of them. The halt is a "soft landing" where the information computed is retained, as the computation will complete the current SCF cycle. Thus, the job may take a few moments to halt execution.

acubegen (new)

Writes a cubefile (Gaussian-style) given a .vis file from an AMPAC calculation. Type "acubegen" followed by return to obtain the quite extensive options for this utility.

minsize (new)

This version of AMPAC uses different size executable images for optimized memory usage. The "minsize" utility examines your data file when you submit a

job and selects which executable is appropriate given the options and the numbers and types of atoms present. The user can also run the utility directly. It takes input from a .dat file and reports the minimum compiled program requirements for running a particular calculation. This information is useful to Semichem Customer Service if a sufficiently large executable is not found.

Suggested usage:
minsize [-v] [-l] file.dat

where "v" provides a verbose listing and "l" provides a listing of the standard program size versions currently installed.

visdump (new)

This utility will convert the binary .vis file to a plain text format for inspection. The output can be quite verbose.

Suggested usage: visdump file.vis | more

arc2dat (new)

Strips the information from a .arc file and writes a .dat file. This utility is useful for running new calculations using previous geometries.

Suggested usage: arc2dat file.arc > file.dat

catcsm (new)

Strips the information from a .csm portable binary file and writes it to an ASCII file.

Chapter 5: New References

COSMO Solvation Model:

Klamt, A. *J. Chem. Soc. Perkin 2* **1993**, 799.

Klamt, A. *J. Phys. Chem.* **1995**, *99*, 2224.

Klamt, A. *J. Phys. Chem.* **1996**, *100*, 3349.

MNDO/d Semiempirical Method:

Thiel, W.; Voityuk, A. A. *THEOCHEM* **1994**, *313*, 141.

Thiel, W.; Voityuk, A. A. *J. Phys. Chem.* **1996**, *100*, 616.

Thiel, W. *Adv. Chem. Phys.* **1996**, *93*, 703.

New CI Method:

Liotard, D.L.; to be submitted.